

Lattice vibrations of α' -NaV₂O₅

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Abstract

We have measured far infrared reflectance and transmittance spectra as well as Raman scattering spectra of α' -NaV₂O₅ single crystals for all the principal polarizations. The temperature range above the phase transition temperature $T_c=35$ K was investigated, mainly. On the basis of this experimental study and of the lattice dynamics calculations we conclude that the symmetry of NaV₂O₅ in the high-temperature phase is described by the centrosymmetric D_{2h} 13 space group. This conclusion leads to important physical consequences concerning the interpretation of one-dimensional magnetic properties of NaV₂O₅ and of the phase transition at 35 K considered earlier to be an ordinary spin-Peierls transition. The assignment of the observed phonons is given. Values of dielectric constants are obtained from the infrared data. Asymmetric shapes of several infrared lines and higher-order infrared vibrational spectra are discussed. The crystal field energy levels of the 3d electron localized at the V⁴⁺ site have been calculated in the framework of the exchange charge model using the values of effective charges obtained from the lattice dynamics calculations. According to the results of these calculations, the broad optical bands observed earlier in the vicinity of 1 eV can be interpreted as phonon assisted d-d transitions. © 1999 American Institute of Physics.
